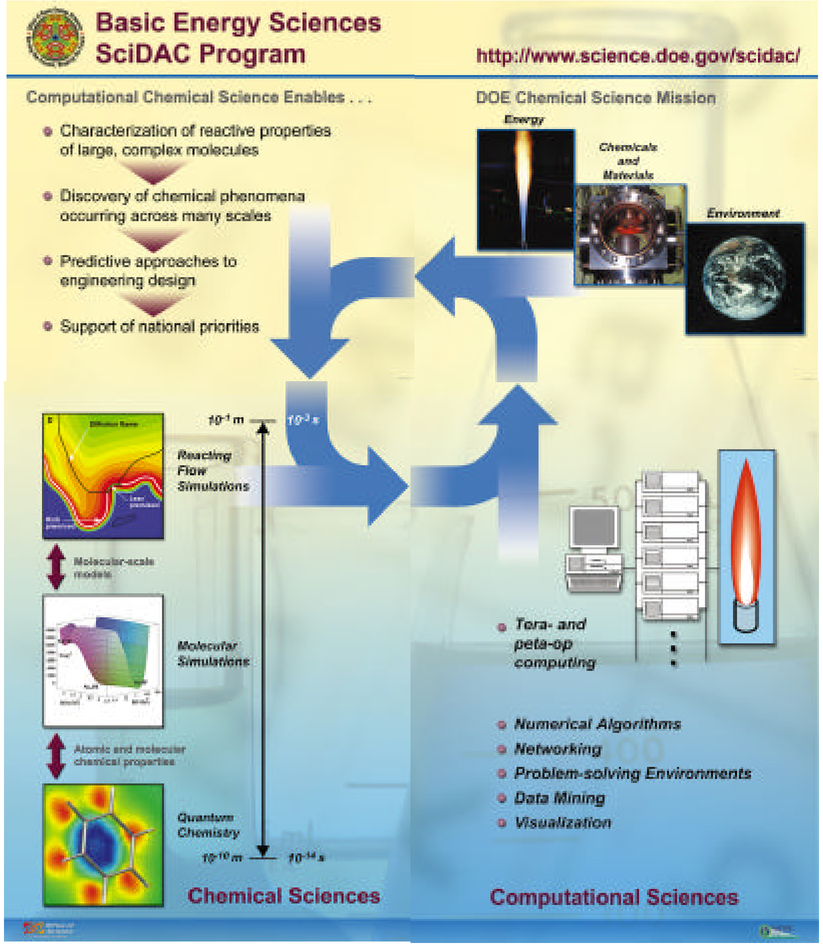
BES SciDAC Computational Chemistry

- Research Goal: *Predictive modeling of important chemical processes*
  - Compute quantum chemistry of large systems
  - Accurately compute properties of open shell molecules
  - Compute properties of turbulent chemically reacting flows
- 13 projects totaling ~ $2M/yr.
- Program management
  - William H. Kirchhoff, DOE
  - Subprogram coordinators:
    - Jeffrey Nichols – Chemistry
    - Larry Rahn – Reacting Flows



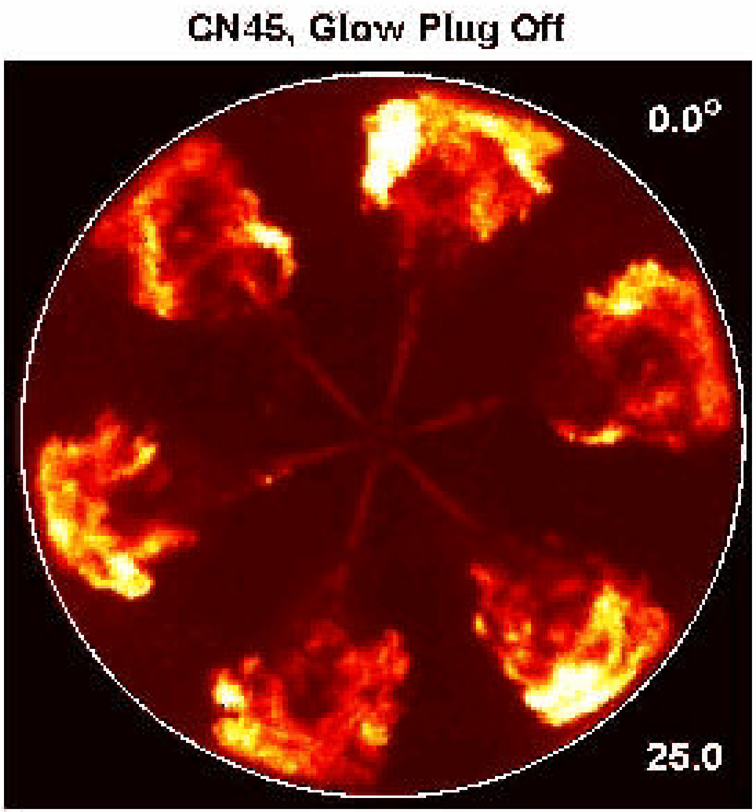
Reacting Flow Science

Larry Rahn, Coordinator

rahn@sandia.gov

SciDAC PI Meeting, March 10, 2003

Challenges in Combustion Modeling

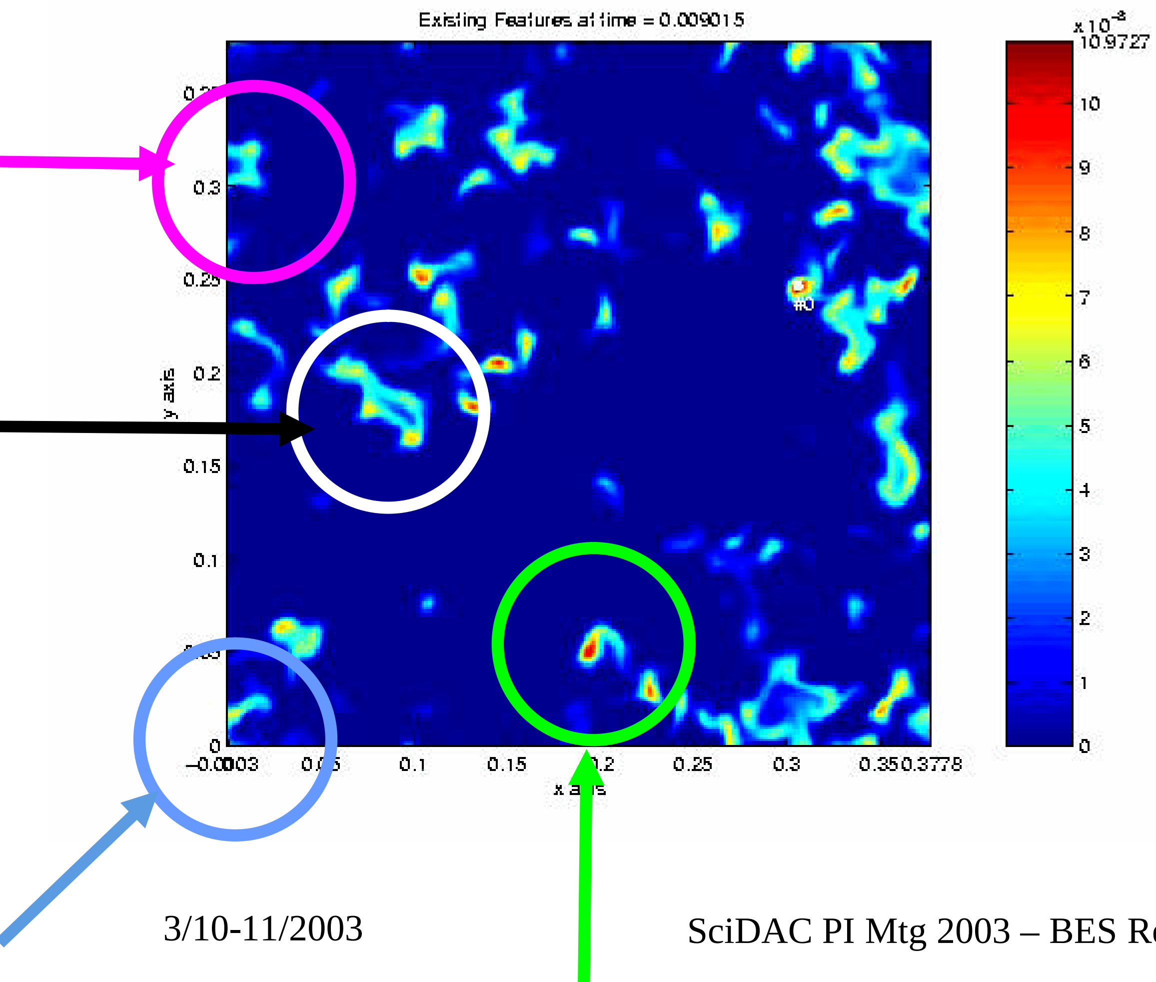


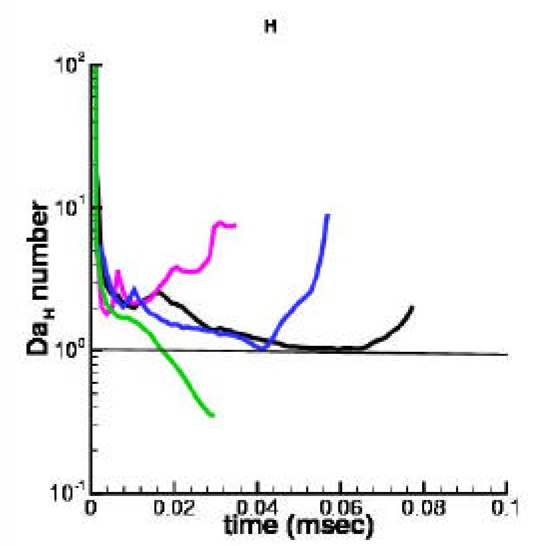
Diesel engine ignition
John Dec, Sandia National Laboratories

- **Stiffness: Large ranges of length and time scales**
  - **turbulence**
  - **flame reaction zone**
  - **high pressure**
- **Chemical complexity**
  - **large number of species and reactions**
- **Physical complexity**
  - **multiphase (liquid spray, gas phase, soot)**
  - **radiation**
  - **acoustics ...**

Autoignition Kernel Survival Criteria Revealed

HO_2 radical evolution from 2D DNS of H_2/air turbulent autoignition



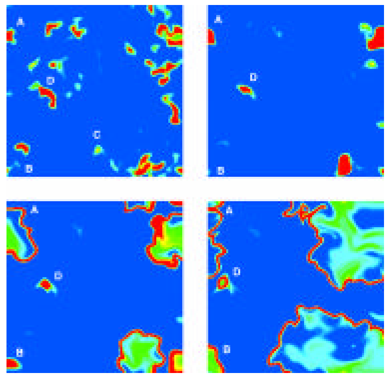


Ignition kernel dies if the time history of the ratio of radical production rate to radical loss rate drops below one.

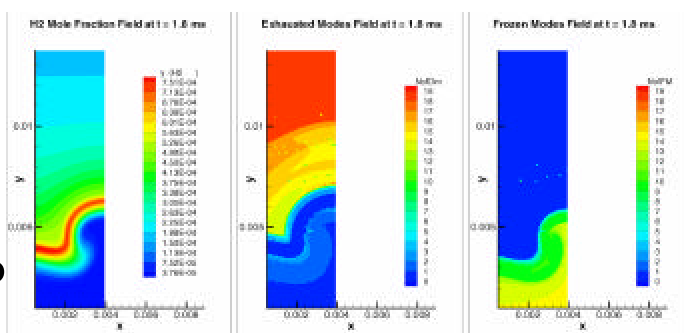
Jackie Chen and Tarek Echekki

SciDAC/BES Reacting Flow Goals

Jet Flame



Autoignition

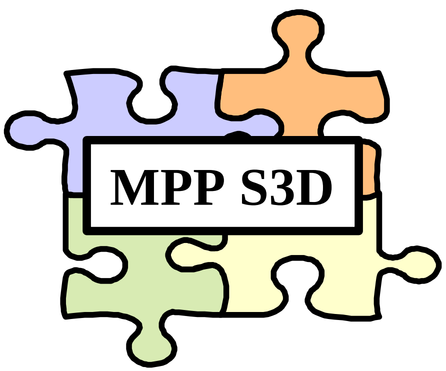


CSP

- Flexible Massively Parallel CCA-based Reacting Flow AMR code and analysis toolkit
- Direct simulation of compression ignition of hydrocarbon fuel
- Direct simulation of NOx in turbulent jet flame
- Chemical analysis in multi-dimensional reacting flow using Computational Singular Perturbation theoryC

BES SciDAC: Reacting Flows Projects

CFRFS



(TSTC)

- **Two Projects Funded at ~ $300k/yr. each**
- **Computational Facility for Reacting Flow Science**
  - **Collaboration of three universities and SNL**
  - Habib Najm @ **PI meeting**
- **Terascale High-Fidelity Simulations of Turbulent Combustion with Detailed Chemistry**
  - **Collaboration of four universities and SNL**
  - Arnaud Trouvé **&** Hong Im @ **PI meeting**

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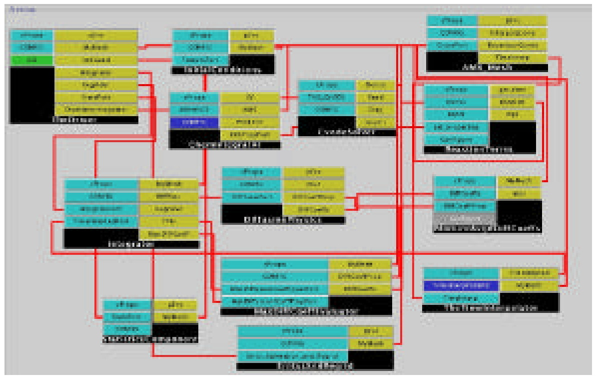
Reacting Flow Strategy & Approach

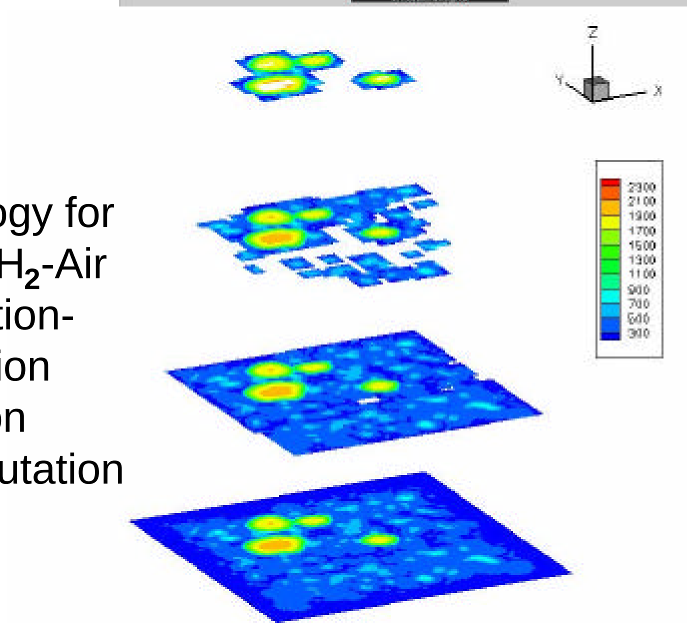
- Implement new architecture enabling collaborative, flexible development of complex MP reacting flow simulation codes
  - **Adopt CCA framework, work with SciDAC ISICs**
  - **Target 3D MP high order Adaptive Mesh Refinement computations of turbulent low Mach number reacting flow**
- Develop new multi-physics, algorithms, and analysis capabilities
  - **Develop CCA-based computational singular perturb. analysis**
  - **Initially target new multi-physics to MPP S3D code**
  - **Integrate new capabilities into CCA MP DNS toolkit**
- Take advantage of new capabilities to accomplish science as they are developed
  - **Initially within the compressible MPP S3D code**
  - **Target grand challenge problems with new codes/computers**

Progress in Software Architecture

CCA GUI showing connections

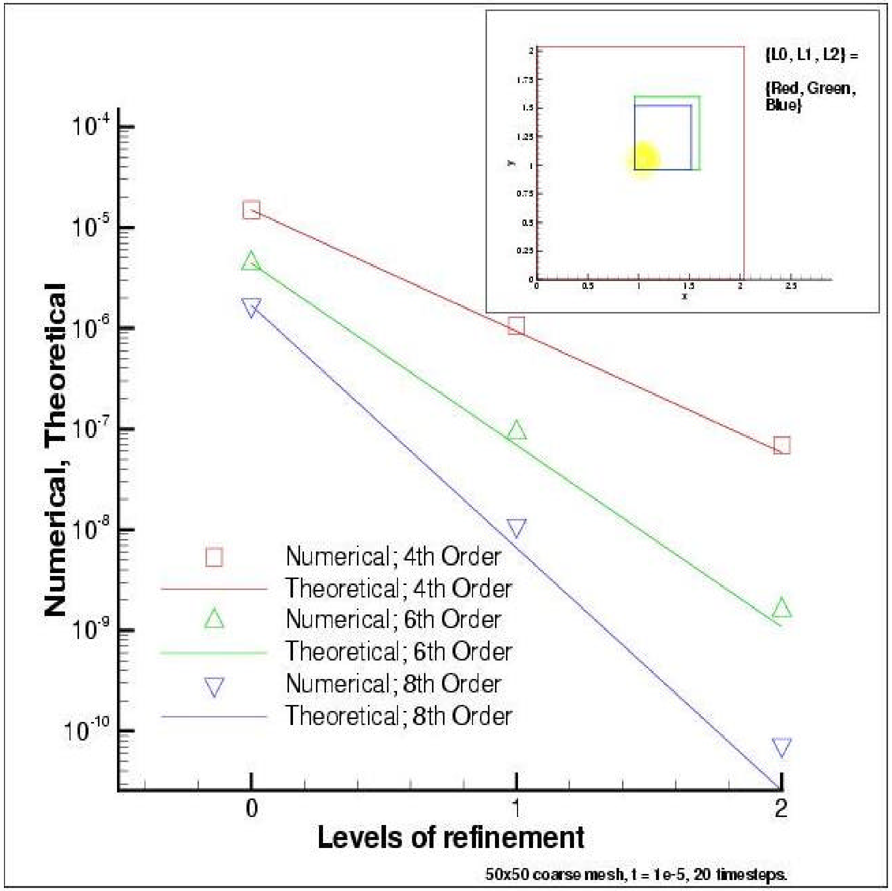


AMR topology for CCA H_2-Air Reaction-diffusion ignition computation



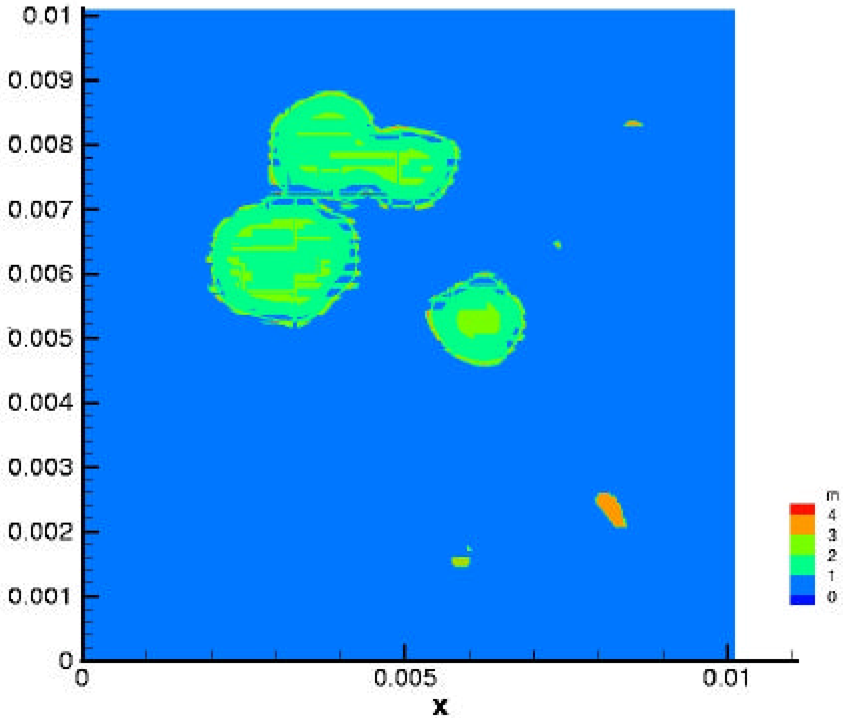
- Thermo-chemistry component
- Transport component
- High-order AMR 3D spatial derivatives and interpolants
- 2nd order Runge-Kutta-Chebyshev (RKC) AMR time integration
- CVODE implicit chemistry integration
- 2nd order operator-split stiff RDR
- Species+Momentum operator-split algorithm
- HYPRE Poisson solve and projection scheme low-M momentum code in progress

High Order AMR



- **Spatial discretizations of first and second derivatives up to 8th order**
- **Boundary conditions and filters up to 12th order, Interpolants up to 8th order**
- **Demonstrated up to 8th order spatial convergence for heat equation on 3 mesh levels**
- **Multi-processor implementation in progress**

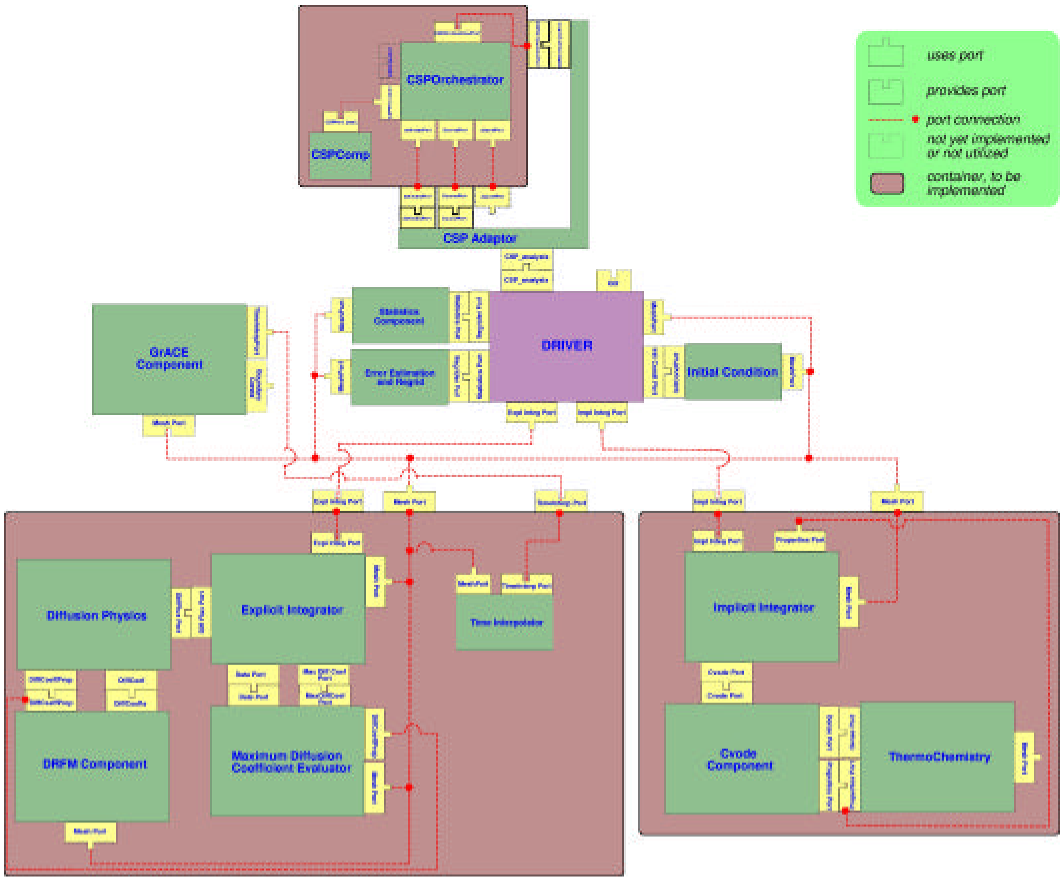
Computational Singular Perturbation (CSP)



Spatial distribution of the number of exhausted modes in CCA/AMR H_2-O_2 ignition

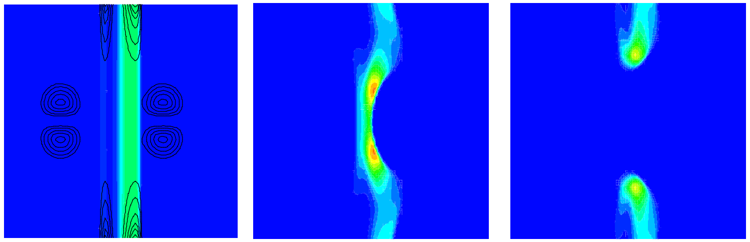
- **Demonstrated use of CSP for analysis of multi-D reacting flow data**
  - **flame-vortex interaction**
  - **CCA/AMR H_2-O_2 ignition**
- **Local equilibrium manifolds and reduced chemical models identified**
- **Identification of cause-and-effect relationships enables extraction of physical insights from data**
- **Second-order spatial errors at mesh patch boundaries**

CCA CSP+AMR-solver Assembly



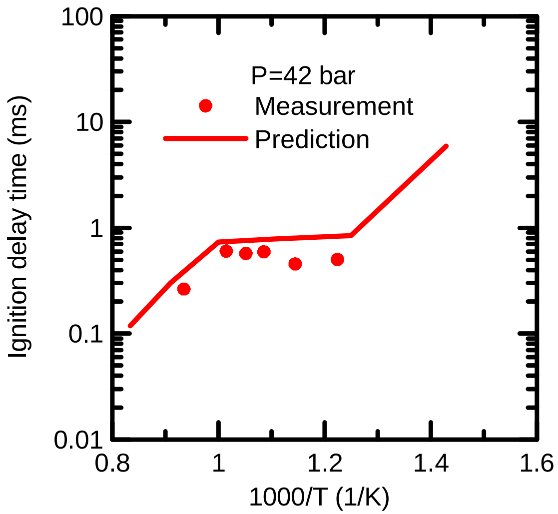
- **Core CSP analysis implemented in CCA & runs online with reacting flow AMR solver**
- **Flexible assembly allows CSP component reuse in alternate code and data analysis CCA constructs**
  - **online or offline**
  - **distributed parallel implementation**

Numerical improvements



Test of the soft-inflow boundary scheme: Vortex-induced quenching in a counter-flow hydrogen-air diffusion flame configuration

Test of the modified chemistry time integrator in a stiff auto-ignition problem

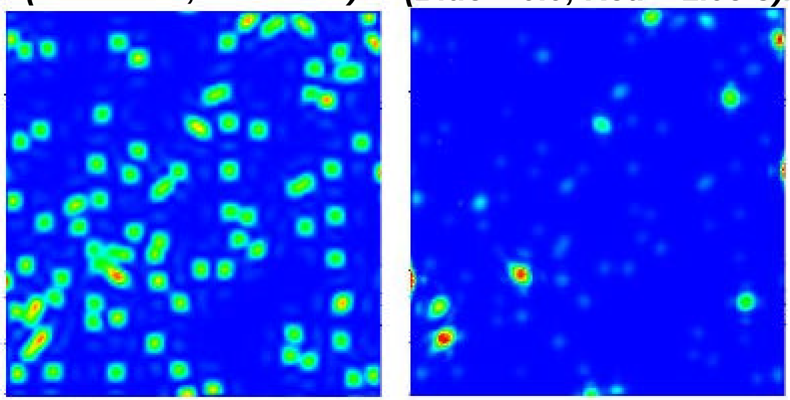


Ignition delay times for n-heptane

- **Implicit/explicit additive Runge-Kutta chemistry time integrator**
- **Pseudo-compressibility method developed for S3D**
- **Inflow boundary scheme modified to improve non-reflecting performance in progress**
- **VODE implicit solver implemented into S3D for auto-ignition problems**

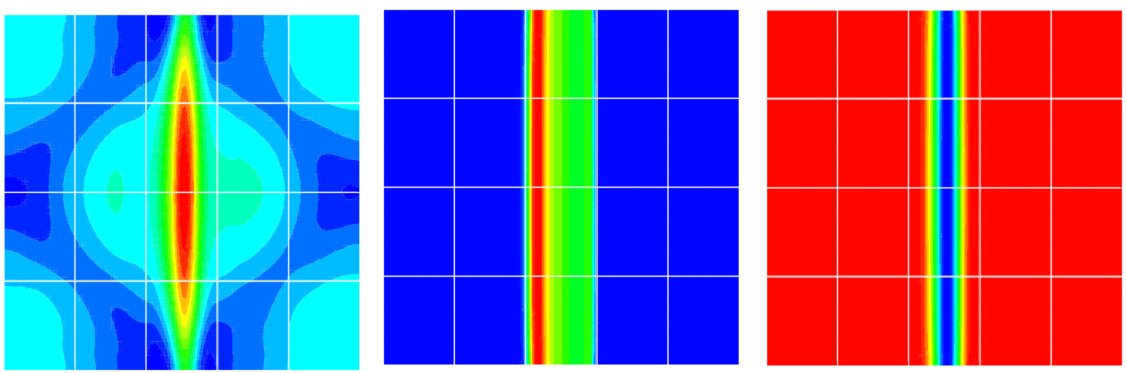
New multi-physics

equivalence ratio (Blue = 0.0; Red = 0.6). *heat release rate (Blue = 0.0; Red = 1.0e-3).*



Test of the liquid spray solver in a turbulent auto-ignition problem

- **Two-equation soot model**
- **4^{th} order Lagrangian particle model for dilute liquid sprays**
- **Discrete ordinate method thermal radiation solver**
- **Discrete Transfer Method radiation solver in progress**



Incident radiation *Absorbed irradiation* *Total radiative power density*

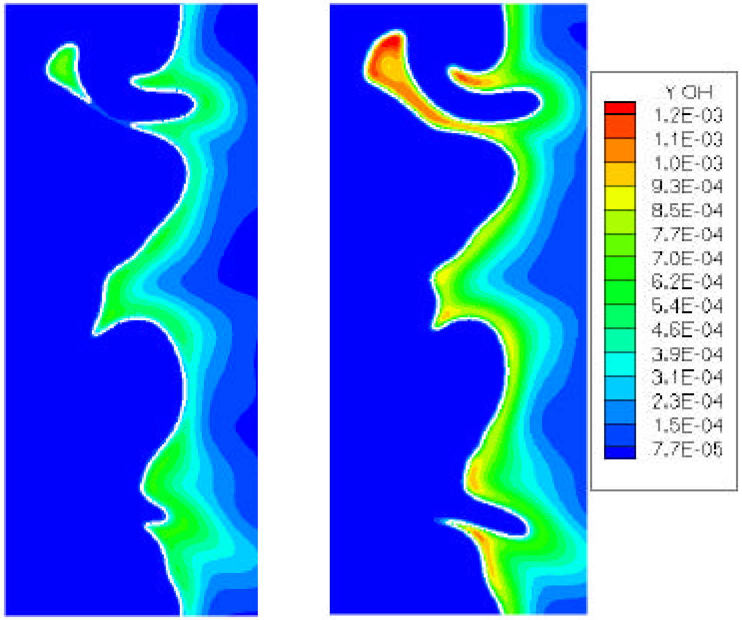
Test of the DOM thermal radiation solver in a laminar counter-flow hrydrogen-air diffusion flame configuration

SciDAC ISIC Collaborations

- CCA - Software architecture
- TOPS - Poisson solvers, stiff integration
- CMCS - Visualization, Feature-tracking
- SDM - Data mining, Feature-tracking

Chemistry-Turbulence Science with S3D

OH mass fraction
Pure CH4-air (Left) ; H2-enriched (Right)



MPP DNS of flame propagation in turbulent premixed hydrogen-enriched lean methane-air mixture

- **laminar flame-vortex interaction in premixed methane-air mixture**
- **turbulent premixed hydrogen-enriched lean methane-air mixture**
- **Turbulent H_2–CO jet flame**
- **Auto ignition in turbulent H_2-air mixture**